

Finite liquid drop size effects on the $d = 3$ Ising simple cubic lattice

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Finite size effects are essential in the study of nuclei and other mesoscopic systems. In cluster physics, finite size effects arise when relating properties of the infinite system to clusters. In nuclear physics finite size effects dominates and the challenge is generalize properties of the nucleus to a description of bulk nuclear matter.

Physical cluster theories of non-ideal vapors, with clusters, state that the concentrations of vapor clusters of A constituents $n_A(T)$ depend on the cluster formation free energy $\Delta G_A(T) = \Delta E_A(T) - T\Delta S_A(T)$. At coexistence, $\Delta E = c_0 A^\sigma$ and $\Delta S_A(T) = \frac{c_0}{T_c} A^\sigma - \tau \ln A$ [1]. Thus

$$n_A(T) = \exp \left[-\frac{\Delta G_A(T)}{T} \right] = q_0 A^{-\tau} \exp \left(-\frac{c_0 A^\sigma \varepsilon}{T} \right) \quad (1)$$

q_0 is a normalization, τ is the topological exponent, c_0 is the surface energy coefficient, σ is the surface to volume exponent, and $\varepsilon = (T_c - T)/T_c$. The term in $\Delta S_A(T)$, proportional to A^σ , permits the vanishing of the cluster free energy at a $T = T_c$. We generalize eq. (1) to the case of a vapor in equilibrium with a finite liquid drop. We extract each vapor cluster from the liquid, determining entropy and energy changes of the drop and cluster, and then put it back into the liquid, as if, according to physical cluster theories, no other clusters existed. Then $\Delta E_A(T)$ and $\Delta S_A(T)$ can be written for a drop of size A_d in equilibrium with its vapor as $\Delta E_A(T) = c_0 [A^\sigma + (A_d - A)^\sigma - A_d^\sigma]$ and $\Delta S_A(T) = \frac{c_0}{T_c} [A^\sigma + (A_d - A)^\sigma - A_d^\sigma] - \tau \ln [A(A_d - A)/A_d]$ giving

$$n_A(T) = q_0 [A(A_d - A)/A_d]^{-\tau} \exp \{ -c_0 \varepsilon [A^\sigma + (A_d - A)^\sigma - A_d^\sigma] / T \}. \quad (2)$$

The free energy cost of complement $(A_d - A)$ formation is determined just as the free energy cost of cluster (A) formation is determined. Equation (2) reduces to eq. (1) when A_d tends to infinity and contains the same parameters. We can rewrite eq. (2) as $n_A(T) = n_A^\infty(T) \exp(A\Delta\mu_{fs}/T)$ with $n_A^\infty(T)$ given by eq. (1). The finite size of the drop acts as an effective chemical potential, $\Delta\mu_{fs} = -\{c_0 \varepsilon [(A_d - A)^\sigma - A_d^\sigma] - T\tau \ln [(A_d - A)/A_d]\} / A$.

To demonstrate this method, we apply it to the canonical lattice gas (Ising) model on the simple cubic lattice with a fixed number of up spins A_d^0 (fixed magnetization M_{fixed} Ising model) [2]. We examine the scaled cluster concentrations: $n_A(T)/q_0 A^{-\tau}$ vs. $c_0 A^\sigma \varepsilon / T$. For M_{free} calculations this scaling collapses cluster concentrations [3]. Finite liquid drop size effects appear in the M_{fixed} cluster concentrations which scale better with eq. (2) than eq. (1). To compare the M_{free} cluster scaling and with the M_{fixed} cluster scaling, we fit the M_{free} clusters to eq. (1) with free parameters T_c , c_0 , σ and τ ;

$q_0 = \zeta(\tau - 1)/2$. See Table I and Fig. 1. Next we calculate χ_ν^2 for the M_{fixed} clusters using eq. (1) and eq. (2) with parameters fixed to the Table I. The M_{fixed} χ_ν^2 values for eq. (2) are smaller than the results for eq. (1) and the data collapse is better.

TABLE I: Fit results

	M_{free}		M_{fixed}				
-	$L \rightarrow \infty$	this work					
χ_ν^2	-	1972					
T_c	4.512 ± 0.001	4.53 ± 0.01					
c_0	≥ 12	12.63 ± 0.04	$A_d^0 (d=3)$	468	234	117	
σ	0.6395 ± 0.001	0.73 ± 0.01	χ_ν^2 eq. (1)	14826	7937	3516	
τ	2.209 ± 0.006	2.26 ± 0.01	χ_ν^2 eq. (2)	1553	839	258	

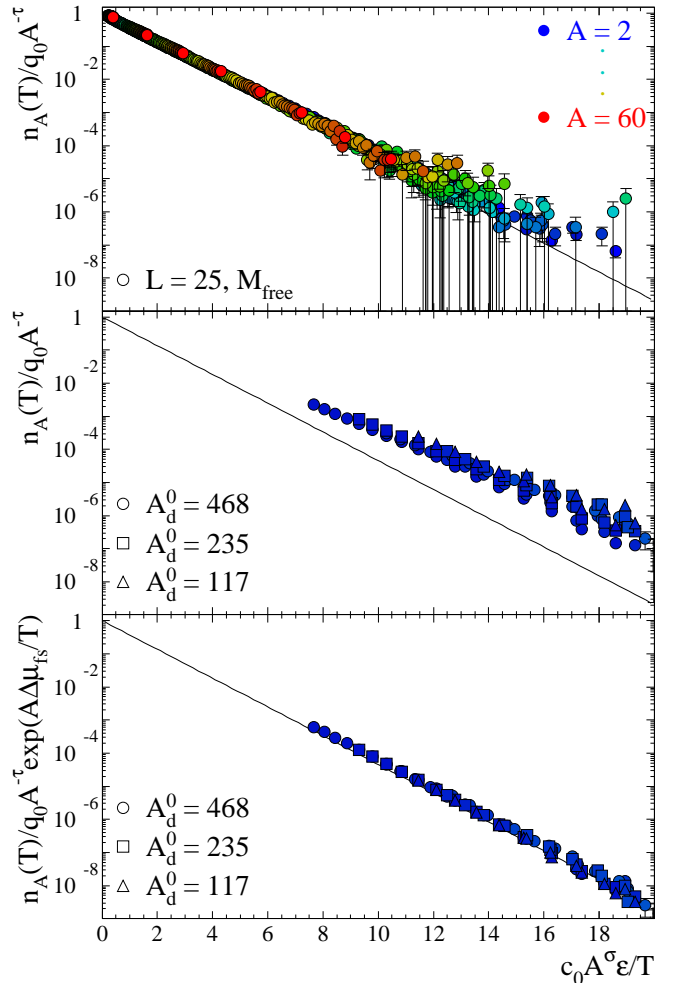


FIG. 1: The scaled cluster yields.

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- [3] C. M. Mader *et al.*, Phys. Rev. C **68**, 064601 (2003).